

UNDERSTANDING MATERIALS RELIABILITY - THE MECHANISMS OF FRACTURE

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ABSTRACT

For the benefit of the NDE community, a personal view will be given of the current status of our understanding of materials fracture. The discussion will include a general description of the physical and chemical processes which occur when a solid under load possesses a crack. A physical picture is presented of the role of plasticity. The basic question of ductile vs brittle response of the solid is addressed and recent ideas and progress reviewed. Time dependence, and its manifestation in materials fatigue are briefly described. The implications for NDE are on two levels: (1) new insight generated by fundamental advances in the science of materials reliability will lead to new NDE tools; and (2) NDE techniques can and should be applied to further the fundamental understanding of reliability.

INTRODUCTION

The NDE community is closely attuned to the problem of finding and characterizing the geometry of flaws in a material, but is normally not involved in the questions which concern the mechanisms by which a material will actually fail. These mechanisms relate to how the stress is concentrated by a flaw, and to the response of the material to the stress and the environment in which the material is immersed. Since it is never a good practice to isolate one aspect of a total technical problem from another, this morning's session is designed to summarize the current status of these other aspects of materials failure.

A PHYSICAL OVERVIEW

Atomic processes are crucial to an adequate understanding of fracture. In this lecture I will address some problems associated with the physical and chemical events taking place at a crack tip where the atomic bonds rupture as the crack advances.

On this most fundamental atom mechanistic level, I know of few more complex sets of phenomena than those involved in fracture. To be specific, a crack is an opening surface interacting with various external and internal chemical environments presented to it. Our problem thus encompasses surface science in both its physical and chemical aspects. However, because a crack is difficult to get at, the powerful techniques which have recently been developed to study highly characterized surfaces are by and large not applicable to the study of fracture. We shall thus have to begin again in the development of more adequate tools to study fracture on a fundamental level.

Second, the atomic structure of the region surrounding the tip is important because the stress at the tip depends upon the positions of these atoms--that is to say whether they are in good material or on a grain boundary containing impurities or precipitates. Hence, fracture encompasses those aspects of solid state physics dealing with solid cohesion. Finally, deformation on a local level and microstructure in the material is crucial, because this determines whether the material is relatively brittle or relatively ductile. Hence, fracture contains most of materials science. Also, all these aspects interact intimately with one another.

In the face of this complexity, our first task is to sort out the basic elements of the problem and decide what are its fundamental aspects.

TABLE I
A Fracture Taxonomy

<u>Prototypes</u>	<u>Material Factors</u>	<u>Fundamental Problems</u>
Brittle Fracture	Plasticity	Ductile vs Brittle
Ductile Fracture	External & Internal Chemistry	Crack Kinetics
	Materials Structure	

Table I, I hope will be helpful as a kind of roadmap in thinking about the subject. There are two prototypes of fracture. The first is the classical brittle fracture in which bonds of the material are progressively broken at a crack tip. The second is fully ductile failure in which the material simply fails by ductile instability. As strain progresses locally, the cross-section of the specimen decreases, which increases the stress progressively until the last atom bond pops. On a localized basis, ductile instability leads to hole growth as depicted in the figures. Figures 1-8 show various aspects of ductile and brittle fracture.

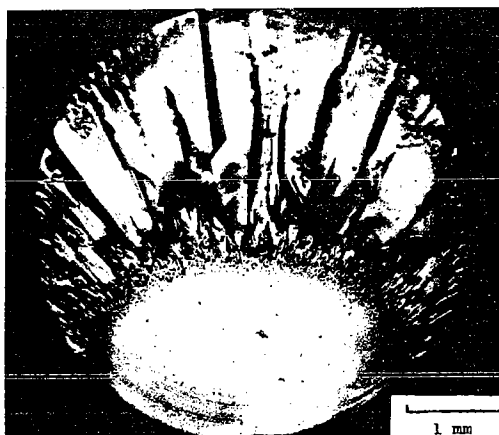


Fig. 1

Brittle fracture of glass. This photo shows the smooth cleavage characteristic of brittle fracture in the lower portion of the photo. The upper half of the cleavage surface is termed "hackle" and is a feature of a fast moving brittle crack. The origin of the fracture was at the bottom of the rod.

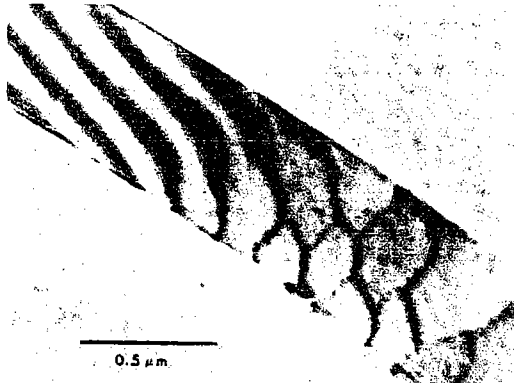


Fig. 2

A truly brittle fracture in Al_2O_3 . In this thin film specimen viewed by transmission electron microscopy, a brittle crack has grown into the material from the lower left, across the field of view, and then receded to the middle of the picture. Misfit dislocations are visible in the upper portion where the crack has healed. The black bands at the bottom are interference fringes across the open crack. (Courtesy of B. Hockey)

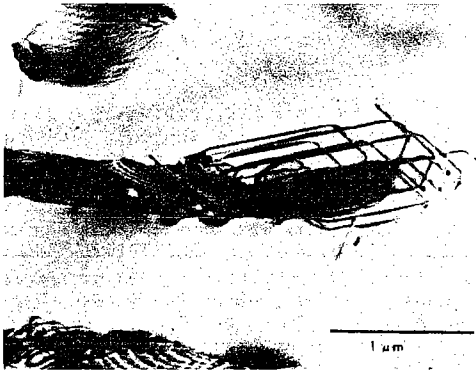


Fig. 3

A partially brittle crack in Si. After the crack grew to the middle of the field of view in this thin film specimen, dislocations were formed around the crack tip as shown. (Courtesy of B. Hockey)

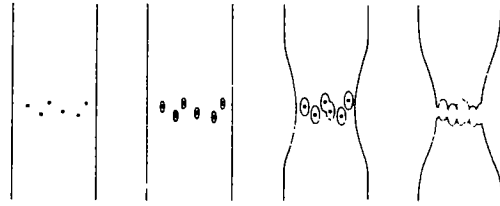


Fig. 4

Schematic view of a specimen in which fracture proceeds by hole growth. Holes are formed at precipitate particles, and under stress, grow until coalescence parts the material into two portions.

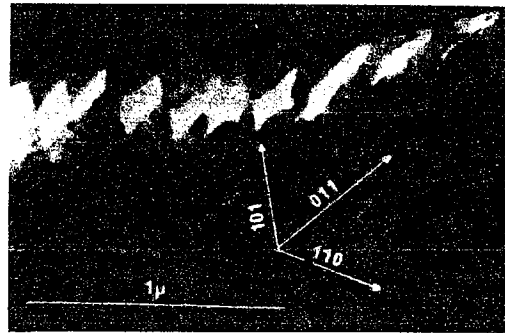


Fig. 5

Hole growth in a thin metal specimen. In this electron microscope picture, the thin specimen nucleates voids ahead of the advancing crack. The specimen fails by coalescence of the voids. (See Ref. 1)

Void Initiation in Ductile Fracture of Metals

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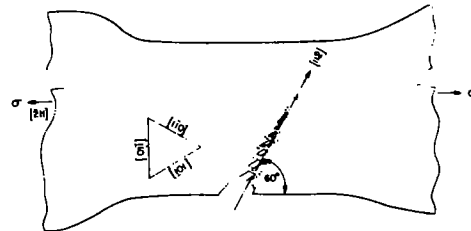


Fig. 6

Schematic view of Fig. 5. (See Ref. 1)

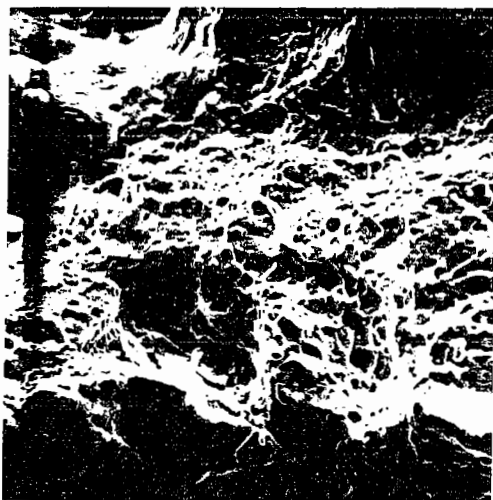


Fig. 7

Fractograph of steel fracture surface showing highly dimpled features characteristic of hole growth mode of fracture



SEM fractograph

1800x

Fig. 8

Fractograph of steel showing intergranular failure. In this case, a brittle crack progressed through the metal along its grain boundaries.

In the second column of Table I, I have listed the most important interactions with other phenomena both external to the material, and internal to it. For example, a brittle crack may emit a dislocation, and be blunted. A continuation of this process would turn a brittle crack into a hole and the brittle crack would disappear. Likewise, external chemical attack at the crack tip may assist the bond breaking process and cause fracture at lower stresses. The interaction of a crack with internal structure may be important as in the case of the grain boundary, where the stress for fracture is again lowered because of both chemical and structural lowering of the interfacial energy.

In the third column of Table I, I have grouped some major problem areas into "fundamental problems". The first is listed as the ductile vs brittle response of a material. In some ways, one can view this as the fundamental problem in fracture, because ductile failure with high toughness is always the most desired materials characteristic. The great surprises occur when the material becomes brittle because of external chemical attack. I imply that when this occurs the underlying fracture type changes from hole growth to brittle. This change of mechanism does not always coincide with the phenomenological transition from ductile to brittle behavior, but is most dramatic when it does--an extreme example is liquid metal embrittlement. I have also listed time dependent fracture effects as fundamental problems because they are kinetic effects, and are not governed by the type of thermodynamic considerations which basically dictate static phenomena.

Table I paints the field of fracture with a very broad brush. None of the topics listed there represents a highly developed and satisfactory body of fundamental knowledge. In the remainder of the lecture, I have time to delve only selectively into a few areas of special interest.

DUCTILE FRACTURE

Let us begin with a brief look at some aspects of the experimental situation in what is perhaps the most important material--steel. Steel is hardly a model material for sorting out the fundamental phenomena in fractures, but it is certainly the most intensively studied.^{2,3} In some very recent experiments, Hirth and co-workers^{2,3} have shown how a crack develops from a broad notch. See Figs. 9-12.

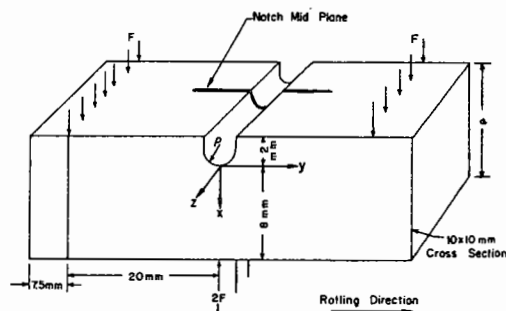


Fig. 9

Schematic of experimental arrangement. The specimen possesses a round notch from which the crack grows under binding stress. (See Refs. 2,3)

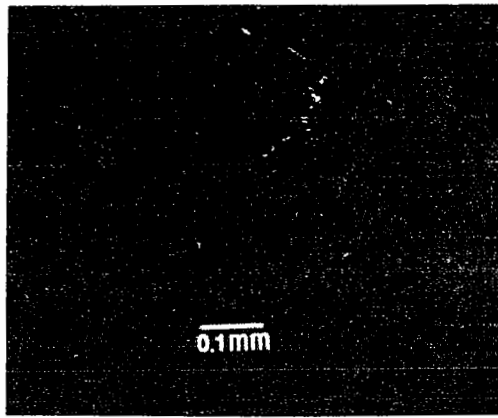


Fig. 10

Ductile fracture follows the curved lines of strain characteristics around the notch. (See Refs. 2,3)

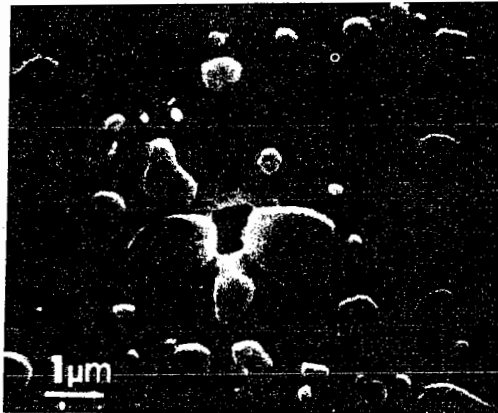


Fig. 11

Hole growth is observed to occur between closely spaced carbide particles in the matrix in the general vicinity of high shear stress. (See Refs. 2,3)

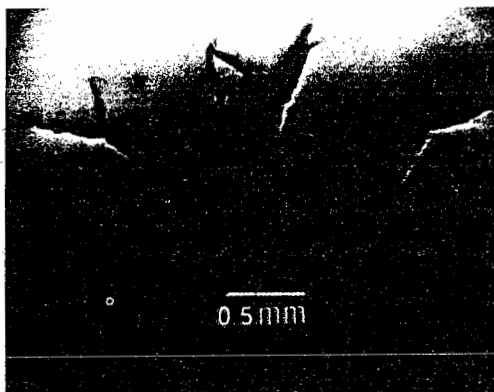


Fig. 12

Brittle fracture proceeds normal to notch surface in presence of hydrogen in high strength steel. (See Refs. 2,3)

A plastic zone develops around the notch, and then a shear instability sets in along the lines coincident with the plastic zone characteristics. In this region of very high localized strain, voids are formed at pairs of hard precipitates where strain incompatibilities are generated. The voids grow by plastic deformation and link up along the shear band, finally opening up into a crack. The effect of hydrogen has been studied, and in soft steels the same process takes place but at lower critical strain. When hydrogen is injected at the notch surface of a high strength steel, however, the whole process changes abruptly. Now a sharp brittle crack initiates at the surface, and grows in the classic fashion into the interior. The action of the hydrogen takes place either at the crack tip, or just inside, near the tip. These experiments illustrate in a beautiful fashion how the same material can exhibit both ductile and brittle fracture under different circumstances, and it illustrates in a straightforward way the important effects which external environments can play.

There are, however, additional chemical effects on fracture which are sufficiently general to be mentioned. Hydrogen not only affects the threshold for catastrophic fracture; it also causes cracks to grow slowly under a steady stress, and it enhances the fatigue failure of steel. Steady state slow crack growth and cyclic fatigue are particularly insidious from a practical point of view, because a part may perform adequately for a long period of time, and yet fail in service because of the undetected growth of cracks to the critical size for sudden failure.

Figure 13 shows the experimental results of Simmons, Wei, and their co-workers on hydrogen in steel. The observed stress dependence is characteristic of all chemically assisted fracture. Also,

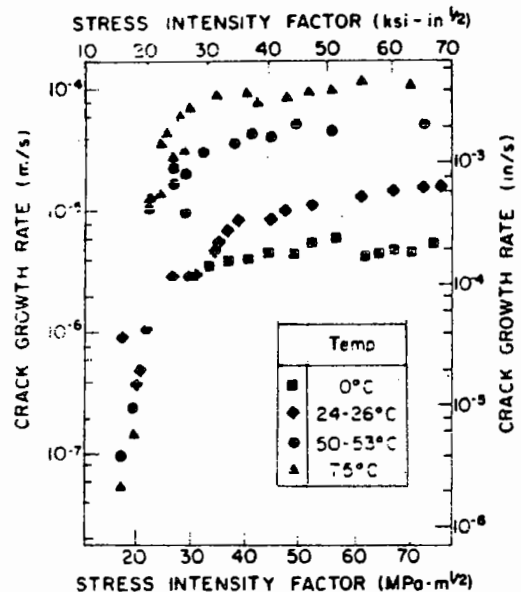


Fig. 13

Crack growth rate as a function of stress intensity factor. (See Ref. 4)

thermal fluctuations are important, and hydrogen shows an activation energy of about 0.15 eV for crack growth in Stage II. Since hydrogen is almost immediately adsorbed on clean iron surfaces, we can interpret the results as a direct interaction at the crack tip. Likewise, in dynamic fatigue shown in Fig. 14, hydrogen has an effect on fracture in

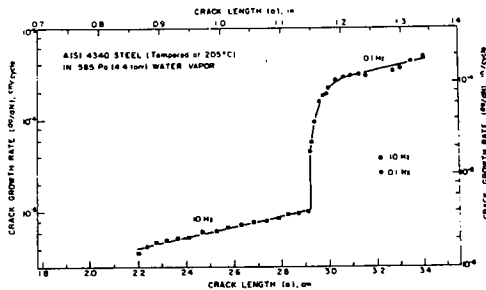


Fig. 14

Crack growth in fatigue is dependent upon frequency of stress cycle. (See Ref. 4)

high strength steel. Again, the crack growth depends upon both the magnitude of the stress and the temperature, although in this case the fundamental chemical effects at the crack tip are more obscure than for slow crack growth.

CHEMICALLY ASSISTED FRACTURE

With this sketchy experimental background, let us now turn to theory, and attempt to build some models which may help bring a measure of physical and chemical understanding to materials fracture. To begin, we focus on the problems of chemical kinetics at a crack tip, and for the moment I will ignore the role of plasticity. Consider the broadest possible picture of a crack which grows from one lattice position to the next by chemical adsorption. Figure 15 shows the configuration space of the entire system

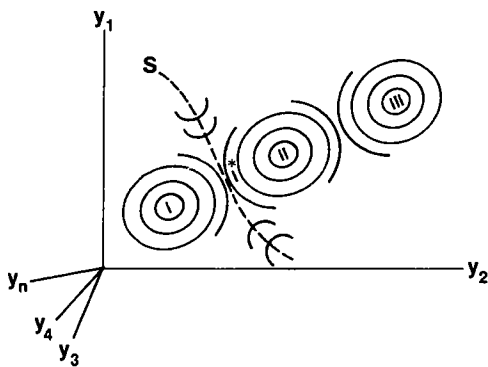


Fig. 15

Configuration space of a cracked material under stress and in presence of external environment. The successive local minima corresponds to crack growth by one atomic unit.

including the external chemical atmosphere. We shall assume that there are a series of local minima in this space corresponding to successive atomic positions of the crack. The rate, v , with which the system transverse a saddle point from one minimum to the next is given by a very simple expression,

$$v = \frac{kT}{h} \frac{Z(I^*)}{Z(I)} \quad (1)$$

where Z is the partition sum of the entire system including the external interacting chemical environment. If we assume that the external chemical environment is a gas of diatomic molecules, and that the material is a vibrating crystal lattice, these partition sums can be computed in principle. We shall assume that when the gas interacts with the crystal, it adsorbs on the surface, and that at the saddle position, one gas molecule interacts with the single breaking bond at the tip. With these assumptions, we can write a formal equation for the crack growth rate. However, I shall not burden you with it. Rather, from this approach we can get some interesting insight into the crack equilibrium condition. For a quiescent crack, we have equal forward and reverse reaction rates, and

$$v(\text{forward}) = v(\text{backward})$$

$$\frac{Z(I^*)}{Z(I)} = \frac{Z(I^*)}{Z(II)} \quad (2)$$

so the intermediate states in I^* cancel out. Since the partition sums are simply related to the free energies, F , of the system, we have at equilibrium

$$F(I) = F(II), \quad (3)$$

which is a thermodynamic statement one might almost have written down without going through the kinetics. We can carry through a transition to the macroscopic quantities one would measure in the laboratory, and when this is done, we have the familiar relation first derived by Griffith,

$$G = 2\gamma \quad (4)$$

where G is the crack extension force, and γ is the surface energy.

The important interpretation of this result is that the equilibrium crack is governed by thermodynamics. We need to know nothing about the detailed force laws of the solid atoms or the external chemical environment to find the stable crack length. This crack length is governed solely by thermodynamic variables such as the surface tension of the solid, chemical potentials of the external gaseous molecules, and the crack extension force. This result was correctly stated by Griffith⁵, by Petch⁶, and more recently by Rice⁷, but is still not properly understood in the fracture community.

Chemical effects are universally thermally activated processes, and we next inquire about activated processes in fracture. You will not be surprised that I shall not get too realistic about such activation energies, but it is instructive to develop qualitative models. For this purpose, consider a two-dimensional array of atoms, Fig. 16.

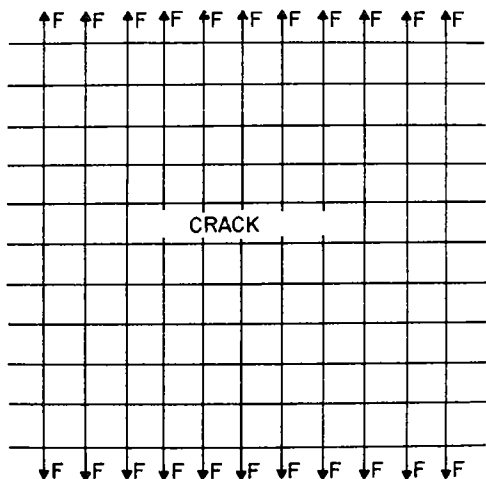


Fig. 16

Two-dimensional array of atoms stressed at outer boundaries and containing a crack.

Assume for the moment that the atoms are all connected with linear springs. Then the solution for a crack of length l is as shown in Fig. 17. When the crack is one atom spacing longer, $l+1$, the compliance is slightly lower, and the slope of the solution in Fig. 17 is likewise lower. For a given length, as

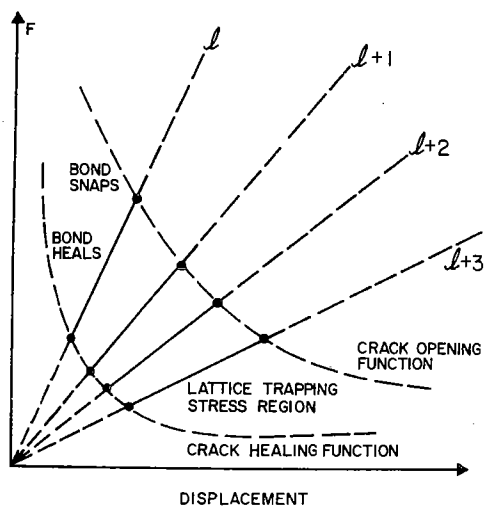


Fig. 17

Solution of two-dimensional array. Force is plotted as a function of displacement of central atom pair. Since forces are linear, solution is a set of straight lines, one for each length, l , of crack.

the stress is increased, the force on the bond at the tip increases until it can no longer hold. The bond breaks, and the solution snaps from one line to the next in Fig. 17. But we can also get from one line to the next by thermal fluctuations. Simple expressions can be derived for the activation energy for one dimensional models of cracks.

The chief conclusions from considerations such as these are: (1) the important chemical assistance to fracture comes from direct interaction at the crack tip; (2) activation energies appear to go as

$$\Delta E \propto (K - K_c)^n \quad (5)$$

where K is the stress intensity factor for the crack. n takes values from about 1.5 to 2; (3) chemical bridging reactions at the crack tip are possible and could have the effect of chemically strengthening a material; (4) molecule size factors can be important in chemically assisted fracture; (5) as in all surface chemistry reactions, chemical specificity will be important; and (6) chemically assisted fracture will have a different (although often analogous) chemistry from plane surface chemistry.

THE ROLE OF PLASTICITY

Recently, three investigators have addressed the effect of plasticity in brittle fracture in a fundamental way^{10,11}. They have all made the assumption that a brittle crack can coexist with a surrounding cloud of deformation without blunting. Figure 18 shows that if the plastic strain surrounding the crack tip is heterogeneous and limited, then

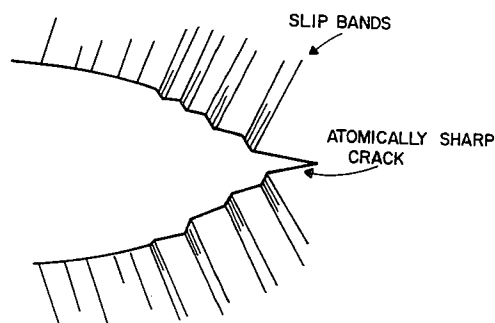


Fig. 18

Schematic drawing of a sharp crack in heterogeneous deformation field. The slip lines are visible on the crack surfaces.

a sharp crack will in fact not be blunted. One can then solve the stress problem, Fig. 19, assuming that the sharp brittle crack which we have just discussed sets the boundary condition for small distances.

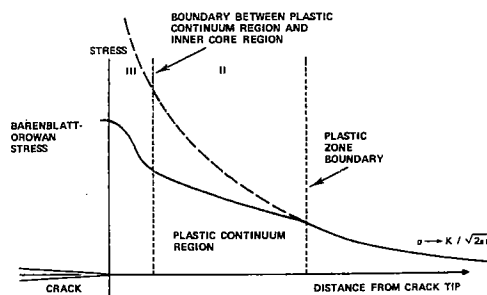


Fig. 19

Schematic view of the stress as a function of distance from a sharp crack embedded in a field of plastic deformation.

Some kind of continuum plastic region is formed in the intermediate region, and at large distances from the crack tip where the stress is below yield, an elastic solution is valid. One can then derive expressions in which the true surface energy of the core crack is a driving term for the whole stress distribution. One such expression predicts that the overall stress intensity factor, K , of the fracture is related to the intrinsic surface energy of the system by

$$K \propto K(\gamma, \sigma_y, \mu, n, \eta) \quad (6)$$

where n is the work hardening exponent, σ_y the yield stress, μ the modulus, and η the maximum density of dislocations at the crack tip. This theory appears to be consistent with the hydrogen embrittlement of high strength steels. The most important conclusion of the work of these three investigators is that a total theory of fracture is given which encompasses a fracture criterion, which is a missing ingredient in any continuum treatment. These theories indicate how the small effects--energywise--which go on at the crack tip of the brittle crack become magnified by the shielding effect of the plastic zone. In further work it will be necessary both to test the range of validity of these ideas, and to give them a more quantitative basis by means of the study of the response of small regions under inhomogeneous high stress. A fundamental understanding of how brittle fracture can become ductile is yet to be developed.

In summing up, from the fundamental physical and chemical point of view, we can begin to see how some of the basic fracture phenomena can be understood in a semi-quantitative way, but this field is characterized by much debate. A great deal of work remains to be done on model systems in order to sort out the elementary processes.

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SUMMARY DISCUSSION
(Robb Thomson)

George Herrmann (Stanford University): Just a point of information on relationship 3. How do you obtain it?

Robb Thomson: One carries through, through the program I just described. The problem is broken into three parts. The inner part consists of a brittle crack, perhaps even in a discrete lattice, there might also be chemistry affecting the crack tip. Then a cutoff radius is defined separating the inner region from the next, intermediate, region described by continuum plasticity. I really don't know how to do that, but results of experiments may eventually help. Of course, this difficulty brings up the whole question of whether the crack tip is blunted by the deformation or not. So, the intermediate region is easy, and the solution for it has been contained in the literature for some time. You can find it, for example, in Rice's article in the Fracture Treatise, Vol. II, even including work hardening. Finally, the third region is the linear region, that portion of the material where the stress is below the yield stress. When these three regions are pasted together, self-consistently, a fracture criterion can be derived.

George Herrmann: From which you derive this expression:

Robb Thomson: Yes. I must say, however, that several people have been deriving fracture criteria for quasi-ductile fracture from slightly different points of view. In addition to the one I have outlined, Wertman, Howard, and Hart have derived such expressions.

Don Thompson (Science Center): I was wondering, when you go through your models and discussion as you have, could you prioritize the properties that one could measure to give an early indication of impending crack growth?

Robb Thomson: You are bringing me down to earth. Well, that's actually going to be the subject of much of the latter part of the morning. It involves a study of the range of slow-crack growth. It involves a study of the threshold values for crack growth; all this is from the empirical point of view. And, of course, it involves a vast amount of study of the understanding of these things. The deeper understanding of fracture is what I have been talking about here. Although, I have tried to indicate where some progress in fundamentals is being made, this understanding has not reached a very complete stage yet in terms of the material factors that govern fracture threshold values and the crack growth values. And, as I indicated, there is a great deal of complexity that goes into the chemistry of the surface and the crack tip regions and the substructure at the crack tip. So, we are a long way from being able to have a very close relationship between the problems you want solved and fundamental understanding.

Unidentified Speaker: Simply a comment on your point 3 to which George Herrmann reacted. That point was made in 1963 by Bertram Grover, namely, the shielding of the plasticity onto the crack tip, and the fact that the intrinsic fracture energy may play a much more important role than has been believed so far. As a matter of fact, I think it was Orowan who suggested that plasticity and intrinsic fracture energy be additive quantities in the fracture process. It turns out in other dissipated materials, such as visco-elastic materials can show very clearly both analytically and experimentally that the two are not additive; they are multiplicative. So, if you make the intrinsic fracture energy zero, you have no strength, as it should be, and you cannot derive simply from plasticity strength. And what the dissipated characteristic does, it modifies the intrinsic fracture energy of the material. So, if you play around with the intrinsic fracture energy of the material, keeping the plasticity aspect, displacing it changes the strength of the material.

Robb Thomson: I couldn't have said it better.

Jim Rose (University of Michigan): What are the physical mechanisms that would lead to the shear crack tip?

Robb Thomson: Well, that's the question which I neither had time to discuss; nor does anybody know much about it. I view ductile fracture and brittle fracture as a competition between two completely different mechanisms. One is a completely plastic process. The other is true fracture, where atoms are pulled apart at a sharp crack tip. The factors which govern how one process overwhelms the other constitutes the fundamental problem which I listed in the beginning of my lecture.

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